

4-Bromo-5-methoxy-3-[(propan-2-yl)oxy]-N-(2H-tetrazol-5-yl)thiophene-2-carboxamide
113589-05-2 | DTXSID60556730

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 327 °C

Global applicability domain: Outside

Local applicability domain index: 1.20e-01

Confidence level: 7.07e-01

Nearest Neighbors from the Training Set

Image not found

Ametryn

Measured: 345

Predicted: 341

Image not found

Desmetryn

Measured: 345

Predicted: 341

Image not found

Auramine

Measured: 331

Predicted: 349

Image not found

3-Methyl-1-phenyl-1H-pyrazol-5-amine

Measured: 333

Predicted: 334

Image not found

2,4,6-Tricyano-1,3,5-triazine

Measured: 262

Predicted: 264